Heptanedioic acid
111-16-0 | DTXSID5021598

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.02e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.91e-01

Confidence level: 5.88e-01

Nearest Neighbors from the Training Set

Image not found
Piperazine
Measured: 9.00e-08
Predicted: 7.31e-01

Image not found
Cycloheptanone
Measured: 2.88e-07
Predicted: 1.00

Image not found
Diallylamine
Measured: 3.18e-07
Predicted: 27.5

Image not found
3-Methylbutyl acetate
Measured: 1.07e-08
Predicted: 6.64

Image not found
2-Ethoxyethyl acetate
Measured: 5.55e-08
Predicted: 1.46